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14. ABSTRACT
1. We have developed methodologies for solving Boltzmann and Fokker-Planck equations using sparse grids and sparse spectral representation. This began as a joint project with Jie Shen, but since it is mainly in his area of expertise, he has been the main driving force behind the implementation.
2. We have used sparse representation to drastically expand the capabilities of the sequential multiscale modeling. We used it calibrate the empirical potentials used in molecular dynamics.
3. We have developed effective sampling methods for very high dimensional stochastic problems in which the noise has a small amplitude but dominant effect.

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Overcoming the curse of dimension: Methods based on sparse representation and adaptive sampling

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1 Introduction and motivation

A major issue in modeling and computation is how to handle high dimensional problems. We can divide these high dimensional problems into two classes: Moderately high dimensional problems or very high dimensional problems. In the former class, we have problems such as the Boltzmann equation, whose dimensionality is high but they are still amendable to grid-based methods. In the latter class we have problems such as exploration of the configuration space of a large molecule. These problems often involve hundreds of thousands of dimensions, and methods based on fixed grids are far from being adequate. We have explored various ways of handling these problems using the sparse representation or the adaptive sampling.

2 Solving Boltzmann and Fokker-Planck equations

Boltzmann equation is one of the most fundamental problems in physics. Fokker-Planck equations have also received a great deal of interest in recent years, particularly in the chemical engineering community, in the context of studying complex fluids.

From a numerical viewpoint, a common difficulty is that dimensionality. For example, Boltzmann equation is usually a 7 dimensional problem, 6 space dimensions plus time. Therefore traditional grid-based methods are ineffective. The method of choice has been Monte Carlo method.

Monte Carlo method suffers from two difficulties. One is the slow convergence rate. The other is the numerical noise in the solutions. For this reason, it is still highly desirable to develop effective grid-based methods that solve directly the partial differential equations.

In collaboration with Jie Shen, we have formulated such a method using sparse representation, including sparse grids and sparse spectral methods. The method is quite promising in the sense that it provides an effective technology for solving intermediate dimensional partial differential equations.

Since the work falls mainly in the domain of expertises of Jie Shen, the subsequent program has been carried out mainly by him, together with our joint post-doc Haijun Yu. Please refer to his report for the progress made in this direction.

3 Exploring parameter space using sparse representation

3.1 Calibrating and improving empirical inter-atomic potentials

One of the most important issue in atomistic modeling is to determine the inter-atomic potential. The process of that often works as follows. One first specifies a form of the potential, based on experience or known facts. This often involves many undetermined parameters. One then determines the value of these parameters using experimental data or data obtained from first principle calculations. Needless to say, the success of such empirical potentials depends heavily on the assumed form.

Assess the accuracy of such an empirical potential is a rather difficult task since the dimension of the configuration space of the atoms is usually quite huge. One question the PI has pursued, in collaboration with physicists Gang Lu at the California State University at Northridge, is to assess the validity of the embedded atom model in the elastic regime. The embedded atom model is a very popular model for studying metallic systems. The space of elastic deformations is parametrized by the strain, which is a 6 dimensional space. Using sparse representation in 6 dimensional space, the PI and collaborators were able to systematically explore the space of elastic deformation. It was found that the embedded atom model works quite well when the system is under shear or tension, but it works quite poorly when the system is under compression. In analogy with the modeling of exchange-correlation functionals in density functional theory and viewing the embedded atom model as the analog of the local density approximation (LDA), the PI and co-workers have developed an analog of the generalized gradient approximation (GGA). Current results suggest that this improved model gives much better results in all regimes. The results are published in [1].

3.2 Sequential multiscale modeling

Sequential multiscale modeling has certain advantages. For example, it does give us a model to work with, not just for computational purposes, but also for analytical purposes. On the other hand, it if often believed that suquential multiscale modeling is limited to the passage of a few parameters from microscale models to macroscale models. If the unknown component of the macroscale model is a function that depends on many variables, sequential multiscale modeling stops being effective. This is generally true. However, the power of sequential multiscale modeling can be greatly improved if sparse representations are used. For example, assume that we are modeling complex materials or complex fluids, for which the constitutive law for the stress is either a function of the strain or the rate of strain, which in three dimension is a function of 6 variables, then it becomes feasible to

precompute the constitutive information using sparse representation. This is illustrated in [2].

This has important consequences in multiscale modeling: In many cases, it is enough to use sequential multiscale modeling if we represent the constitutive information in a smart way.

4 Exploring very large dimensional configuration space using adaptive sampling

Sparse representation is only effective if the dimension of the problem is only moderately high. In computational science we often encounter problems whose dimension can be thousands or even larger. In this case, we have to use other strategies.

One strategy that we have pursued so far is adaptive sampling. The general procedure is as follows. We first identify a lower dimensional region (e.g. points, curves or surfaces) in the configuration spaces. We then sampling the probablity distribution of our interest in the neighborhood of that region, and determine how the region moves in the iteration. Such an adaptive sampling procedure has been used with great success to gradient systems, i.e. systems that have an underlying energy landscape, with applications to many important problems in material science, chemistry and biology.

Our new interest is to study non-gradient systems, of which fluid dynamics is a good example. For that purpose, we will proceed in a number of steps. We will use transition pathways between stable states as an example.

4.1 The adaptive minimum action method

Given two stable or metastable states, we would like to find the most probable transition path between the two states. For gradient systems, the string methods have been very successful. For non-gradient systems, we are exploring the mimimum action method, which is more general, but to be effective, it requires a high quality mesh along the path in order to resolve the path. This is very important since these paths are often very complicated. The PI and collaborators have developed an adaptive minimum action method. The basic idea comes from the moving mesh method. The objective is to find the optimal mesh using carefully chosen monitor functions, as the iteration proceeds. This is very simple, but it proves to be quite effective [3].

4.2 Application to the KS equation

As an application, the PI and co-workers have used the adaptive minimum action method to study the dynamics of the Kuramoto-Sivashinsky equation in its configuration space. One first identifies a stable stationary solution and another traveling wave solution. By finding transition pathways between these two solutions, one further finds more stationary solutions. More importantly, one can further refine the whole procedure and find important objects on the separatrices between the basins of attractions of the different stable

solutions. This procedure gives us a rich set of information about the very complicated configuration space of the Kuramoto-Sivashinsky equation. The results are documented in [4].

The example studied so far is the Kuramoto-Sivashinsky equation. But the methodology is fairly general.

We are in the process of applying this methodology to study noise-induced instability and transition to turbulence in incompressible fluids. We have made some initial progress, but this is a very difficult problem and much work remains to be done.

References

[1] G. Wu, G. Lu, C.J. Garcia-Cervera, and W. E, Density-gradient-corrected embedded atom method, Phys. Rev. B, 79, 035124 (2009).

[2] C.J. Garca-Cervera, W. Ren, J. Lu, and W. E, "Sequential multiscale modeling using sparse representation", Comm. Comp. Phys., 4(5), pp. 1025–1033 (2008).

[3] X. Zhou and W. Ren and W. E, "Adaptive minimum action method for the study of rare events", J. Chem. Phys., 128, 10, 2008.

[4] X. Wan, X. Zhou and W. E, "Noise-induced transitions in the Kuramoto-Sivashinsky equation", preprint, submitted.